7-Amino-4-hydroxynaphthalene-2-sulfonic acid 87-02-5 | DTXSID7026520

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.683

Global applicability domain: Inside

Local applicability domain index: 4.48e-01

Confidence level: 5.21e-01

Nearest Neighbors from the Training Set

Image not found

2-Amino-1-naphthalenesulfonic

acid

Measured: -1.16 Predicted: -0.766

Image not found

2-Naphthalenesulfonic acid, 1-

amino-

Measured: -0.970 Predicted: -0.767

Image not found

4-Amino-1-naphthalenesulfonic

acid sodium salt Measured: -2.34 Predicted: -1.01

Image not found

1-Naphthalenesulfonic acid, 5-

hydroxy-

Measured: -0.170 Predicted: -0.435